FCT Fundação para a Ciência e a Tecnologia

Computação Científica Nacional
FCCN

BOB
Operation Report

FCT supercomputing cluster installed at MACC.

October, 2020

EXECUTIVE SUMMARY

BOB is a supercomputing cluster donated by TACC to FCT and installed at MACC. It was inaugurated in July 2019, beginning at that time its pilot and testing phase.

During the period under review in this report, a restricted set of entities were invited to participate, to validate the basic set of computational services and to achieve operational stability.

In the absence of a dedicated operational team, this pilot phase was accomplished by the joint effort and dedication of collaborators from the following entities: FCT, UMinho, INESCTEC, LIP and INCD.

By the end of 2019, tune-ups and troubleshooting were carried out, especially with the storage sub system, a high-performance data storage system whose final configuration stabilized in December.

During the pilot it became evident the inability of Riba d'Ave data centre to ensure total cooling needs for BOB, as well as the unavailability of NOS to improve its facilities for this purpose. This represents a limitation of 35% in the computing capacity of BOB, persisting to the present time. There was also a refusal to respond to requests for quotations to upgrade the current 1 Gbps NOS connectivity, or to install low level transmission operator services.

It was also found that the age of the computing equipment, around 8 years old, leads to a high rate of failures that impacts the stability of computational services.

With all the contingencies and difficulties of the pilot phase, and to avoid a negative user experience, the initial enrolment of new users was performed gradually and without widespread publicity.

This report shows that even with all the contingencies and difficulties encountered in this initial phase, the capacity used in BOB has had a sustained growth, having registered in September a utilization of more than 50% of the available capacity. During the pilot, over 32 million core-hours of processing time took place, involving more than 20 user entities from north to south of Portugal, covering various areas of knowledge. This is a result that is considered highly encouraging and validates the great usefulness of this type of resources, as well as the national capacity to use them.

Currently, due to an increase in the number of orders received, it was necessary to start implementing a quota policy to try to ensure fairer models of access to the computational resources.

The pilot will end with the evolution of BOB usage to more formal processes of access transparency and service security, which are being finalized through a set of administrative instruments, such as FCT's regulation for access to computer resources and the operational support agreements, essential to frame the offered services.

FCT has already taken the first step in the next operational stage of BOB, by opening a public call for access to computer resources for the scientific community and is currently on the process of evaluating the proposals and deciding on computational resources attribution.

CAPACITY USAGE

The operational computational system contains 8,320 CPU cores, which corresponds to 6 million potential core.hours of processing capacity available each month, not considering the time for BOB maintenance. The total computational system made available by TACC would be capable of providing 9.3 million core.hours per month, free from the cooling limitations referred previously.

Definition of core.hour = processing hours multiplied by the number of processing units used in parallel. Term commonly used in Supercomputing as a unit for quantifying CPU usage. This general definition may have variants in the general definition if, instead of using generic CPU, specialized units are used, such as GPU. Each microprocessor may have several CPU cores. For example, in each node of the BOB HPC cluster, there are two CPUs, each with 8 cores.

The following graph shows BOB's capacity utilization in September 2020:

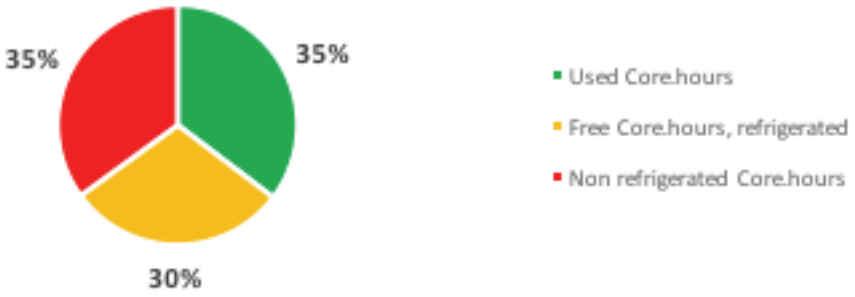

Figure 1 – Bob usage profile

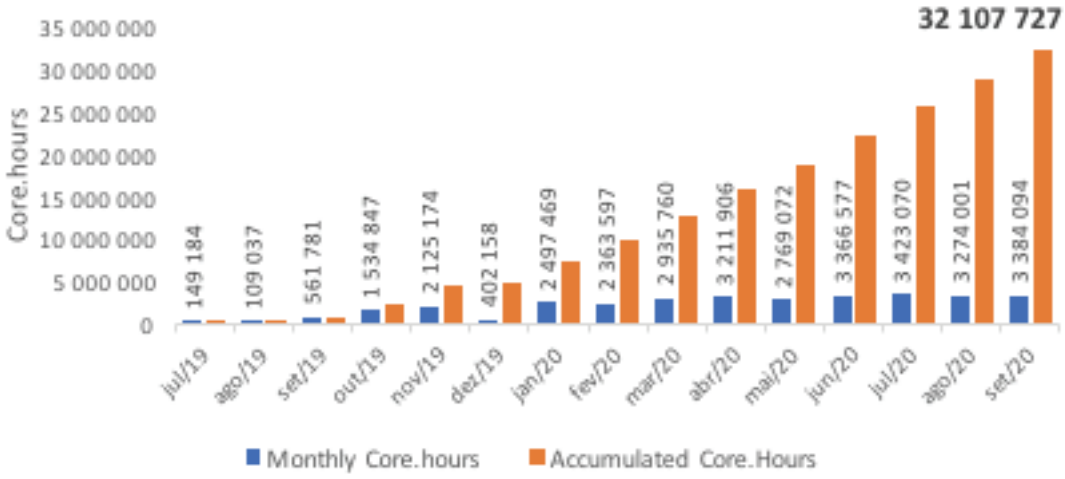

Figure 2- Monthly usage evolution, from July 2019 to September 2020.

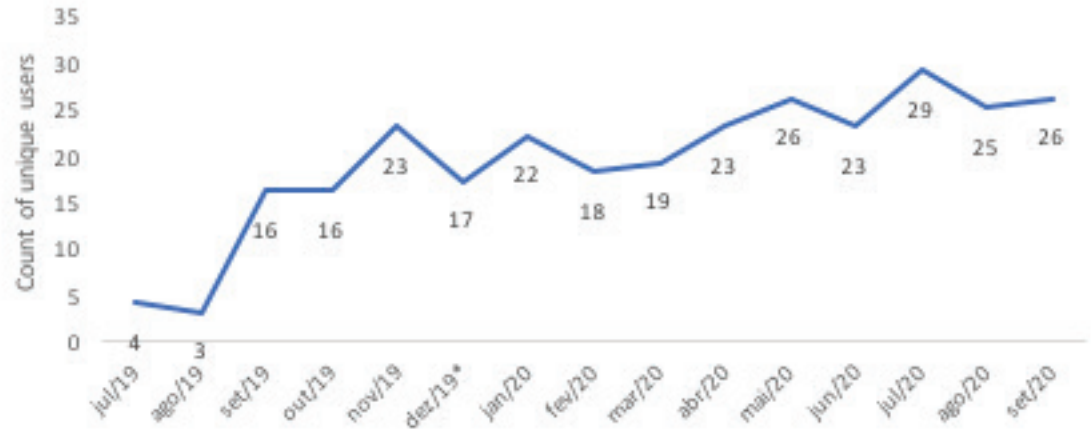

Figura 3 - Monthly evolution of the number of distinct users, from July 2019 to September 2020. Each point represents the number of different usernames - by project or by institution - that used the machine in that month.

(*) In December 2019 the storage system upgrade took place which led to a general system shutdown. The following graph shows the consumption of core.hours per user institution until September 2020.

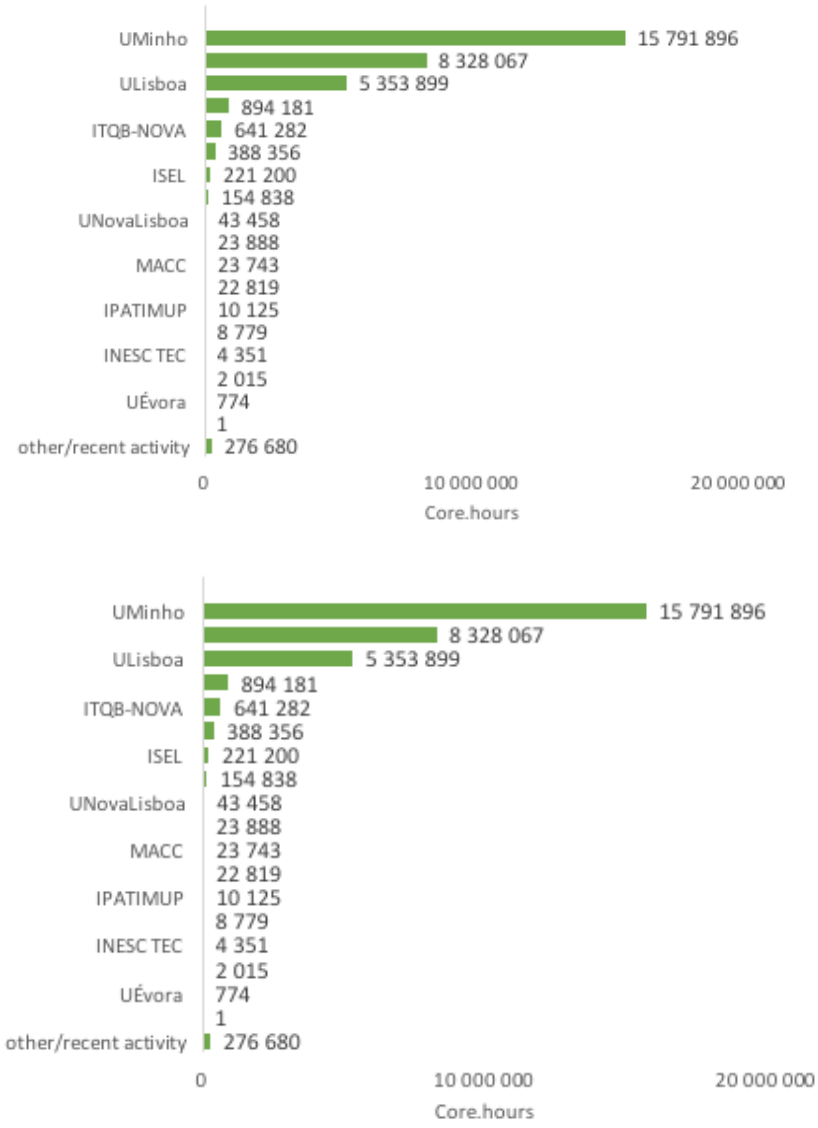

Figura 4- Number of core.hours per institution from July 2019 to September 2020. Acronyms in detail in Table 1.

The “other / recent activity” bar represents usage for which user questionnaires have not yet been received. The following graph shows the consumption by region, according to the user institution.

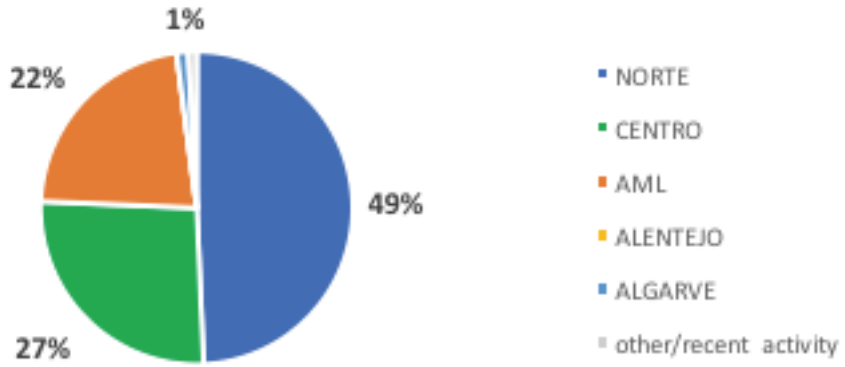

Figure 5 - Percentage of core.hours by region NUT II from July 2019 to September 2020. AML – Área Metropolitana de Lisboa.

The following graph shows consumption by scientific areas, from July 2019 to September 2020:

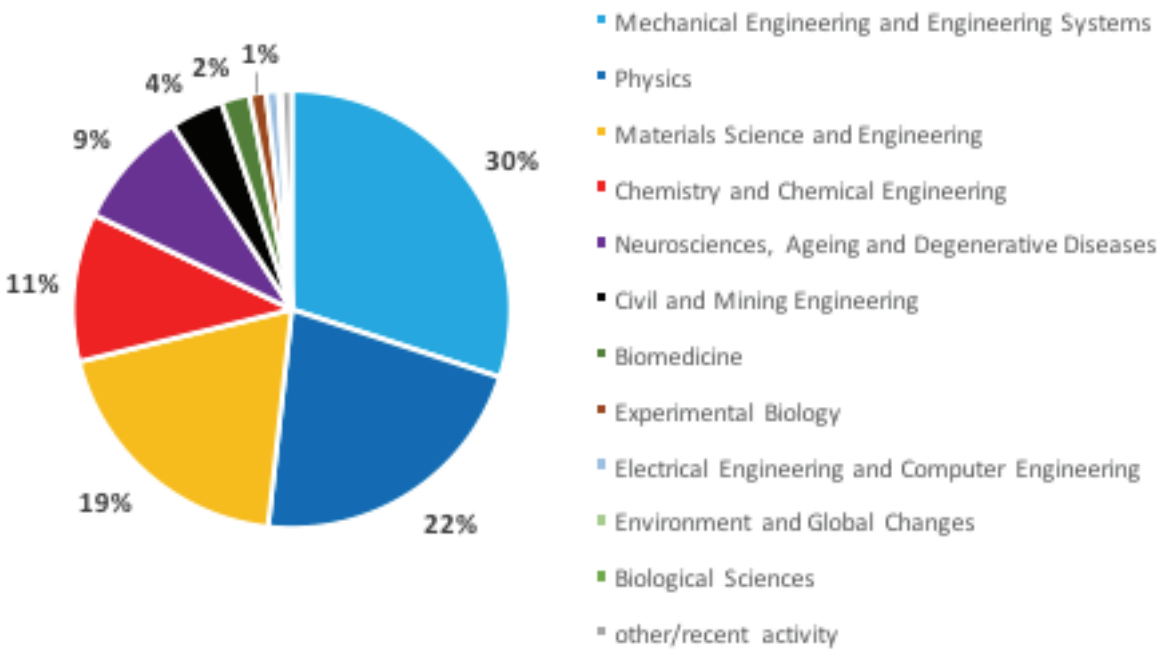

Figure 6 - Percentage of core.hours used by scientific area between July 2019 and September 2020

Note: The information presented is based on user surveys conducted in March and April 2020. In the absence of a specific answer, the scientific area was estimated through the affiliation of the projects or users.

The following tables lists the requested computational projects.

TABLE 1 | USER INSTITUTIONS FROM JULY 2019 TO SEPTEMBER 2020:

Region NUT II	Institution	Subject	Scientific Areas
NORTE	UMinho - Universidade do Minho	Polymers engineering	Materials Science and Engineering
			Mechanical Engineering and Engineering Systems
	LIP - Laboratório de Instrumentação e Física Experimental de Partículas	Physics	Physics
	INESCTEC - Instituto de Engenharia de Sistemas e Computadores, Tecnologia e Ciência	Genetics	Biological Sciences
	DTx - Digital Transformation CoLAB	Several	Electrical Engineering and Computer Engineering
	INEGI - Instituto de Ciência e Inovação em Engenharia Mecânica e Engenharia Industrial	Several	Mechanical Engineering and Engineering Systems
CENTRO	CICECO - Instituto de Materiais da Universidade de Aveiro	Materials science	Chemistry and Chemical Engineering
	UC - Universidade de Coimbra	Neuro inflammation; Drug discovery	Neurosciences, Ageing and Degenerative Diseases
			Chemistry and Chemical Engineering
		Neuroscience and Cell Biology	Neurosciences, Ageing and Degenerative Diseases
		Physics	Physics
		Physics,Lattice	Physics
ÁREA METROPOLITANA DE LISBOA (AML)	UL - Universidade de Lisboa (Técnico)	Mechanical engineering	Mechanical Engineering and Engineering Systems
		Plasmas and Nuclear Fusion	Physics
	UL - Universidade de Lisboa (FCUL)	Molecular Dynamics	Chemistry and Chemical Engineering
	IDL - Instituto Dom Luiz	Climate change	Environment and Global Changes
	ISEL - Instituto Superior de Engenharia de Lisboa	Machine Learning and Optimization Problems	Electrical Engineering and Computer Engineering
	LNEC - Laboratório Nacional de Engenharia Civil	Hidraulics, Coastal modelling	Civil and Mining Engineering
			Environment and Global Changes
	FCT-UNL – Faculdade de Ciências e Tecnologia da Universidade Nova de Lisboa	Molecular chemistry	Chemistry and Chemical Engineering
	ITQB-UNL - Instituto de Tecnologia Química e Biológica	Biotecnology	Biological Sciences
	ISQ – Instituto de Soldadura e Qualidade	No information, Recent activity	Materials Science and Engineering
ALENTEJO	UE -Universidade de Évora	AstroPhysics	Physics; Maths
ALGARVE	UALG - Universidade do Algarve	Genetics	Biological Sciences
VÁRIAS REGIÕES	EDP	Energy	Electrical Engineering and Computer Engineering
	Vestas	Energy	Electrical Engineering and Computer Engineering

SWOT ANALYSIS

After having finished the experimental operation cycle and BOB's trials, it is important to perform a brief SWOT analysis of the entire system, in order to support management decisions, of something that is currently the biggest computational resource of RNCA – National Network of Advanced Computing.

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